Exponentially consistent K-means clustering algorithm based on Kolmogrov-Smirnov test

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Motivation

- non-parametric
- continuous distribution
Notation

- $K = 3$ - # of distributions
- $M = 15$ - # of sequences
Kolmogrov-Smirnov (KS) distance

- Empirical c.d.f. - \( F_x(a) = \frac{1}{n} \sum_{i=1}^{n} 1_{[\infty,a]} x_i \)
  - \( x = \{x_1, \ldots, x_n\} \) - data sequence
  - \( 1_{[\infty,a]} \) - indicator function

- KS distance:

\[
d_{KS}(\ast, \ast) = \sup_{a \in \mathbb{R}} \left| F_\ast(a) - F_\ast(a) \right|
\]

- \( \ast, \ast \) - sample data or distributions.
Fundamental lemma

Lemma 1 (Massart1990)

Suppose $x$ is generated by $p$ and $F_x(a)$ is the corresponding empirical c.d.f. Then

$$P(d_{KS}(x, p) > \epsilon) \leq 2 \exp(-2n\epsilon^2).$$
Reasonable clustering result given $p_i$'s
Lemma 2

Suppose $x$ and $z$ are generated by $p_1$, and $y$ is generated by $p_2$. Then,

$$P\left(d_{KS}(x, z) > d_{KS}(y, z)\right) \leq 6 \exp\left(-\frac{nd_{KS}^2(p_1, p_2)}{8}\right).$$
Reasonable clustering result with unknown $p_i$'s

Cost function: $J = \sum_{l=1}^{3} \sum_{x_j \in C_l} d_{KS}(x_j, c_l)$
Exponential consistency is established for the proposed algorithm.

- \( P_e \) - the probability of error of a clustering algorithm
- \( n \) - sample size
- Consistency: \( \lim_{n \to \infty} P_e = 0 \)
- Exponentially consistency: \( \lim_{n \to \infty} -\frac{1}{n} \log P_e > 0 \).
Clustering given $K$ - Initialization

**Algorithm 1** KS-based initialization given $K$ for composite distributions

1: **Input:** $\{x_j\}_{j=1}^M$, number of clusters $K$.
2: **Center initialization**
3: **Cluster initialization**
4: **Output:** $\{C_k\}_{k=1}^K$

- Center initialization
  - Maximize the minimal distance [Katsavounidis-etal 1996]
  - Randomly choose [Moreno-Sáez-etal 2014]
Center initialization illustration
Center initialization illustration cont.
Center initialization illustration cont.
Center initialization illustration cont.
Cluster initialization illustration

Cost $J_1^0$
Clustering given $K$ - Iteration

**Algorithm 2** KS based clustering given $K$ for composite distributions

1. **Input:** $\{x_j\}_{j=1}^M$, number of clusters $K$.
2. **Initialization:** obtain $\{C_k\}_{k=1}^K$ by Algorithm 1.
3. **while** the clustering result does not converge **do**
   4. **{Center update}**
   5. **{Cluster update}**
4. **end while**
5. **Output:** $\{C_k\}_{k=1}^K$. 
Iteration one - center update illustration

Cost $J_1^0$
Iteration one - center update illustration cont.

Cost $J_1^1 (< J_1^0)$
Iteration one - cluster update illustration

Cost $J_1^2 (< J_1^1)$
Iteration two - center update illustration

Cost $J_1^3 (< J_1^2)$
Iteration two - cluster update illustration

Cost $J_1^4 (= J_1^3)$
Theoretical result - Algorithm 2

Theorem 1

Algorithm 2 converges after finite number of iterations and the error probability after $T$ iterations is upper bounded by

$$P_e \leq 2M(K^2 + 3(T + 1)(K - 1)) \exp\left(-\frac{nD^2_{KS}}{8}\right).$$
Clustering without $K$

- Question: Is it possible to cluster with unknown $K$
  - Merge [Wang-etal 2018]
  - Split [Mora-López 2015]
Clustering without $K$ - Merge

**Algorithm 3** KS-based initialization with unknown $K$ for composite distributions - merge

1: **Input**: $\{x_j\}_{j=1}^M$.
2: $\{\text{Center initialization with threshold } d_{th}\}$
3: Clustering initialization specified in Algorithm 1.
4: **Output**: $\{C_k\}_{k=1}^\hat{K}$. 
Center initialization illustration
Merge based - center initialization
Merge based - cluster initialization

Cost $J^0_2$
Algorithm 4 KS based clustering with unknown $K$ for composite distributions - merge

1: **Input:** $\{x_j\}_{j=1}^M$.
2: **Initialization:** $\{C_k\}_{k=1}^{\hat{K}}$ by Algorithm 3.
3: while the clustering result does not converge do
4: Center update specified in Algorithm 2.
5: $\{\text{Merge Step with threshold } d_{th}\}$
6: Cluster update specified in Algorithm 2.
7: end while
8: **Output:** Partition set $\{C_k\}_{k=1}^{\hat{K}}$. 
Merge based - center update

Cost $J^0_2$
Cost $J^1_2 (< J^0_2)$
Merge based - merge step

Cost $J_2^2$
Theoretical result - Algorithm 4

**Theorem 2**

Given \( d_{th} = \frac{D_{KS}}{2} \), Algorithm 3 and 4 converges after finite number of iterations and the probability of error is upper bounded by

\[
P_e \leq \left( 4M^2(K + 1) + 6M(K - 1)(T + 1) + 4TK^2 \right) \exp \left( - \frac{nD_{KS}^2}{4} \right).
\]

| 0 < D_{KS} \leq \min_{k \neq k'} d_{KS}(p_k, p_{k'}) |
Numerical Result - Given $K$

- $\mathbf{x}_j \sim \mathcal{N}(\mu, 1)$
- $\mu \in \{0, 1, 2, 3, 4\}$

- $\mathbf{x}_j \sim \mathcal{N}(0, \sigma^2)$
- $\sigma^2 \in \{1, 2, 4, 8, 16\}$
Numerical Result - Without $K$

\[
\begin{align*}
\mathbf{x}_j &\sim \mathcal{N}(\mu, 1) \\
\mathbf{x}_j &\sim \mathcal{N}(0, \sigma^2)
\end{align*}
\]
Conclusion

- Clustering sequences generated by unknown continuous distributions.
  - Upper bound of $P_e$
  - Exponential consistency of $P_e$